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XAS Studies on $ZrO_2/SiO_2/Si$ Gate Stacks for CMOS Applications

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The International Technology Roadmap for Semiconductors foresees an ~1 nm effective gate oxide thickness for 0.1 μm CMOS technology nodes by 2006[1]. In this oxide thickness regime, the use of SiO_2 and SiO_xN_y dielectric layers (below 1.2-1.5 nm) will not be possible for many applications due to intolerable tunneling currents. Therefore the gate dielectric and capacitance scaling have emerged as a critical challenge for future device scaling. One solution being extensively explored is to increase gate capacitance by replacing SiO_2-based dielectrics with higher permittivity dielectrics. For a given capacitance (electrical thickness), a high-K dielectric should show a lower leakage than SiO_2.

ZrO_2 has received considerable attention in last few years as one of the potential replacements for SiO_2 in future CMOS devices, due to its high dielectric constant (16-25) and moderately large band gap (5.4 –6.0 eV) [2-4] Zhao et al [5]have recently reported on the dielectric properties of low-pressure crystal phases of ZrO_2, where they have clearly showed that the dielectric response of the material is strongly phase dependent.

Several different deposition techniques have been utilized for growth of thin films of ZrO_2 including sputtering, chemical vapor deposition, sol-gel based methods, evaporation/re-oxidation and more recently atomic layer chemical vapor deposition. Thin films prepared on silicon by different methods and even from different precursors can result in quite different physical and electronic properties.

In view of the importance of developing an understanding of the crystal and electronic structure of thin ZrO_2 dielectric films on silicon we are performing Zr-$L_{2,3}$ edge XAS on ZrO_2 films deposited by ALCVD (atomic layer chemical vapor deposition) on 10A SiOxNy/p-Si(100). These studies are facilitated by extensive XAS ZrO_2 based compound studies by our group in the past. Preliminary Zr-$L_{2,3}$ results on the thin film materials clearly show well defined spectral features associated with the 4d crystalline field (CF) split empty states. The CF splitting appears smaller in the films as compares to the bulk materials. The fine structure above the Zr-L_3 edge indicates a Zr-O distances typical of the bulk material. Detailed comparison of the XAS results are being made to band structure calculations and inverse photoemission measurements.

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